

Tridecane
629-50-5 | DTXSID6027266

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 5.93

Global applicability domain: Inside

Local applicability domain index: 4.55e-01

Confidence level: 5.41e-01

Nearest Neighbors from the Training Set

Image not found

Tetradecane

Measured: 7.20

Predicted: 7.15

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Dodecane

Measured: 6.10

Predicted: 5.90

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Decane

Measured: 5.01

Predicted: 5.24

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Cyclohexane, dodecafluoro-

Measured: 2.91

Predicted: 3.19

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2-(Tetradecylamino)ethanol

Measured: 5.74

Predicted: 5.67